

FULL ESTIMATED COST

0.63

0.63

FILE 'REGISTRY' ENTERED AT 08:58:33 ON 25 JAN 2006  
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STRUCTURE FILE UPDATES: 23 JAN 2006 HIGHEST RN 872490-64-7  
DICTIONARY FILE UPDATES: 23 JAN 2006 HIGHEST RN 872490-64-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when  
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\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

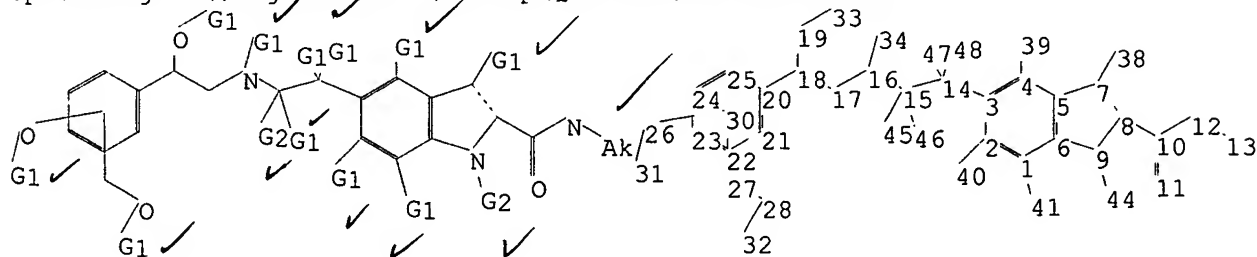
Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10813426\3.str



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chain nodes :
10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 38 39 40 41
44 45 46 47 48
ring nodes :
1 2 3 4 5 6 7 8 9 20 21 22 23 24 25
chain bonds :
1-41 2-40 3-14 4-39 7-38 8-10 9-44 10-11 10-12 12-13 14-15 14-47 14-48
15-16 15-45 15-46 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28 28-32
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24
24-25
exact/norm bonds :
1-41 2-40 4-39 5-7 6-9 7-8 7-38 8-9 9-44 10-11 10-12 12-13 14-47 14-48
15-16 15-45 15-46 16-17 16-34 18-19 19-33 26-31 27-28 28-32
exact bonds :
3-14 8-10 14-15 17-18 18-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25
isolated ring systems :
containing 20 :

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G1:H,CH3

G2:H,Ak

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 38:CLASS
39:CLASS 40:CLASS 41:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS

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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 08:59:01 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 80161 TO ITERATE

100.0% PROCESSED 80161 ITERATIONS  
SEARCH TIME: 00.00.10

L2 54 SEA SSS FUL L1

54 ANSWERS

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL  
SESSION

FULL ESTIMATED COST

166.94

167.57

FILE 'CAPLUS' ENTERED AT 08:59:16 ON 25 JAN 2006  
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FILE COVERS 1907 - 25 Jan 2006 VOL 144 ISS 5  
FILE LAST UPDATED: 24 Jan 2006 (20060124/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

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L3            3 L2  
  
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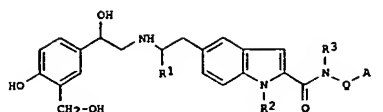
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 ACCESSION NUMBER: 2004:712649 CAPLUS  
 DOCUMENT NUMBER: 141:277488  
 TITLE: Preparation and in vitro activity of novel indole-2-carboxamide  $\beta$ 2-adrenoreceptor agonists  
 INVENTOR(S): Brown, Alan D.; Bryans, Justin; Bunnage, Mark E.; Glosop, Paul; Lane, Charlotte; Mantell, Simon; Lewthwaite, Russell A.  
 PATENT ASSIGNEE(S): Pfizer Limited, UK  
 SOURCE: Eur. Pat. Appl., 58 pp.  
 CODEN: EPAXDX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1460064	A1	20040922	EP 2003-100650	20030314
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CA 2517569	AA	20040923	CA 2004-2517569	20040301
WO 2004080964	A1	20040923	WO 2004-IB591	20040301
WO 2004080964	C1	20050929		
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1611097	A1	20060104	EP 2004-715968	20040301
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US 2004235833	A1	20041125	US 2004-800253	20040312
PRIORITY APPLN. INFO.: EP 2003-100650				20030314
			US 2003-486535P	P 20030710
			WO 2004-IB591	W 20040301

OTHER SOURCE(S): MARPAT 141:277488  
 GI

Instant App

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Title compds. [I, Q = single bond or C1-4-alkyl-substituted C1-4 carbon chain; R1 = H, C1-4 alkyl; R2 = H, alkyl or benzyl (un)substituted by OH, C1-6 (hydroxy)alkyl, C1-6 alkoxy, halo, OCF3, substituted alkylsulfonylamino, SO2NR9R10, CF3, NR9R10 (R9, R10 = H, C1-4-alkyl); R3 = H, C1-6 (hydroxy)alkyl; A = C3-6(hydroxy) (alkyl)cycloalkyl, C5-10 alkyl or (alkyl)amino (un)substituted heterocyclyl, containing 1-3 O, S, N heteroatoms; Ph (un)substituted by OCF3, alkylsulfonylamino, SO2NR9R10, NR9R10, OCHH2Ph, OH, C1-6 (hydroxy)alkyl, C1-6 alkoxy, halo, thio(C1-6)alkyl, CF3, same R9, R10; preferably R1 = Me; R2 = H, Me, Et, CH2Ph; R3 = H, Me; Q = CH2, CH2CH2, CHMe; A = pyridyl, thiazolyl; preferably 18 specific compds.

corresponding to the above definitions, useful as  $\beta$ 2-adrenoreceptor agonists (cAMP EC50 = 0.03-0.75 nM), and their pharmaceutically acceptable acid or base salts, are claimed. Also claimed are an intermediate carboxylic acid and ester, corresponding to definition I and process of preparation of compds. I, comprising coupling of the carboxylic acid with amines R3NHQA (same R3, Q, A). The use of compds. I is claimed for treatment of airway diseases, such as asthma, bronchitis, pneumonia, emphysema, dyspnea, airways hyper-reactivity, pneumoconiosis; central nervous system disorders such as depression, Alzheimer's disease, Parkinson's disease, mental impairment, drug dependence, dementia; premature labor; allergic skin diseases, psoriasis, glaucoma, gastric and peptic ulceration. In an example, O-tert-butylidimethylsilyl derivative of the

(R,R)-5-substituted indole-2-carboxylic acid, corresponding to definition I (R1 = Me, R2 = H), prepared by N-alkylation of Me (2'R)-5-(2-aminopropyl)-1H-indole-2-carboxylate by (oR)-4-PhCH2O-3-HOCH2C6H3CH(OTBDMS)CH2Br, was reacted with 2-CF3O-C6H4NH2 to give, after deprotection, (R,R)-I, (Q =

CH2, A = 2-CF3O-C6H4, R1 = Me, R2 = H).

IT 757963-27-2P 757963-30-7P 757963-33-0P

757963-36-3P 757963-39-6P 757963-41-0P

757963-44-3P 757963-47-6P 757963-50-1P

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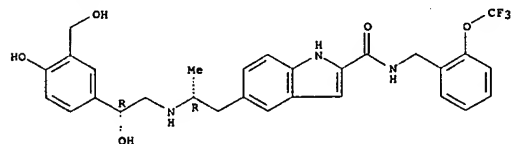
757963-67-0P 757963-69-2P 757963-71-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of 5-aminoalkyl-substituted 2-indole-N-alkylcarboxamides as  $\beta$ 2-adrenoreceptor agonists)

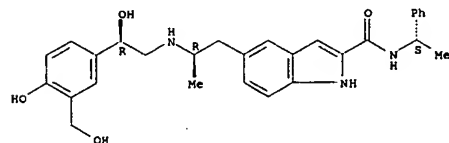
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 CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[[12-(trifluoromethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 757963-30-7 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[[15-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

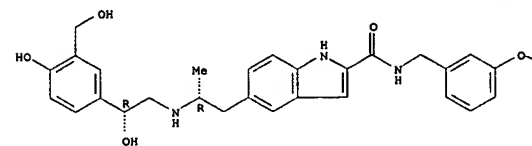


RN 757963-33-0 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[[3-(trifluoromethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

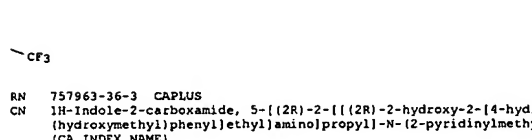
Absolute stereochemistry.

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

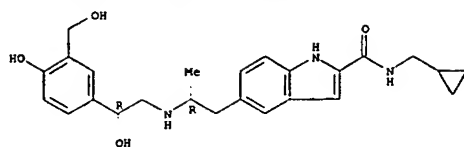


Absolute stereochemistry.

RN 757963-39-6 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-(cyclopropylmethyl)-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

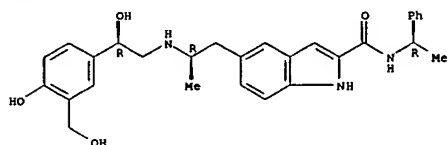
Absolute stereochemistry.

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



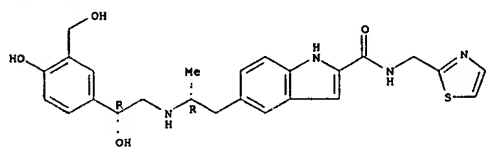
RN 757963-41-0 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(1R)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



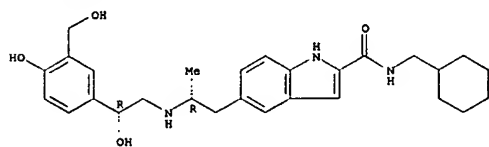
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CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-(2-thiazolylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 757963-47-6 CAPLUS  
CN 1H-Indole-2-carboxamide, N-(cyclobutylmethyl)-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

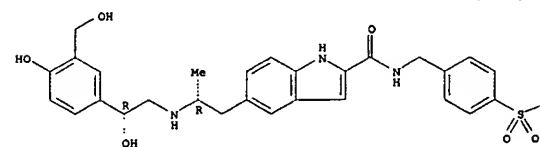
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 757963-56-7 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(4-(methylamino)sulfonyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

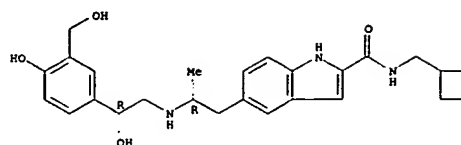
NHMe

RN 757963-59-0 CAPLUS  
CN 1H-Indole-2-carboxamide, N-[(4-(aminosulfonyl)phenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

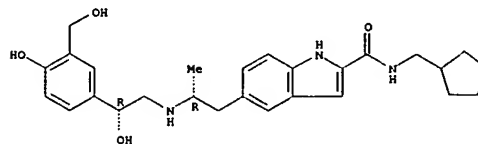
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



RN 757963-50-1 CAPLUS  
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Absolute stereochemistry.

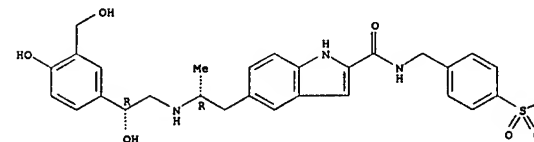


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CN 1H-Indole-2-carboxamide, N-(cyclohexylmethyl)-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A

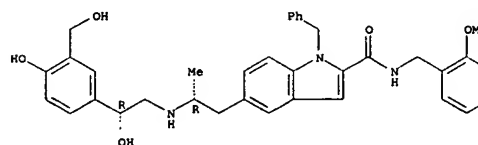


PAGE 1-B

NH2

RN 757963-61-4 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(2-methoxyphenyl)methyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

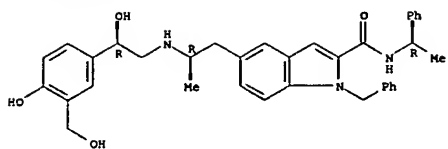
Absolute stereochemistry.



RN 757963-63-6 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(1R)-1-phenylethyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

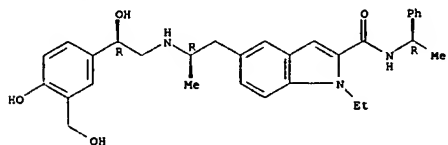
Absolute stereochemistry.

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



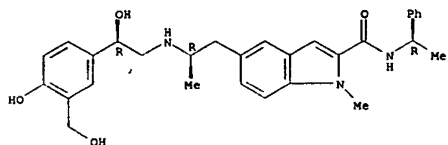
RN 757963-65-8 CAPLUS  
CN 1H-Indole-2-carboxamide,  
1-ethyl-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-[(1R)-1-phenylethyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



RN 757963-67-0 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-1-methyl-N-[(1R)-1-phenylethyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



RN 757963-69-2 CAPLUS  
CN 1H-Indole-2-carboxamide,  
N-[(2,6-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI)  
(CA INDEX NAME)

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:333571 CAPLUS  
DOCUMENT NUMBER: 140:321235  
TITLE: Preparation of indolecarboxamides as  $\beta$ 2 adrenergic receptor agonists  
INVENTOR(S): Brown, Alan Daniel; Bryans, Justin Stephen; Bunnage, Mark Edward; Glossop, Paul Alan; Lane, Charlotte  
Alice Louise; Lewthwaite, Russell Andrew; Mantell, Simon John  
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.  
SOURCE: PCT Int. Appl., 110 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

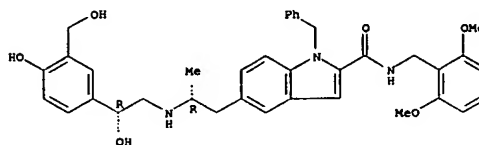
*Inventors*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1556034	A1	20050727	EP 2003-751095	20031006
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NO 2005001406	A	20050422	NO 2005-1406	20050317
PRIORITY APPL. INFO.:			EP 2002-292513	A 20021011
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OTHER SOURCE(S): MARPAT 140:321235  
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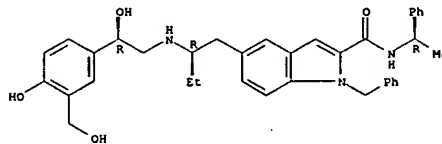
L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

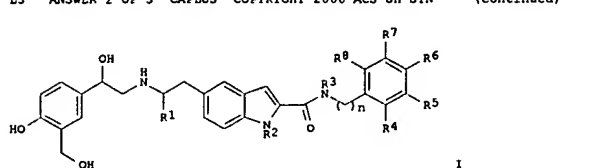


RN 757963-71-6 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]butyl]-N-[(1R)-1-phenylethyl]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



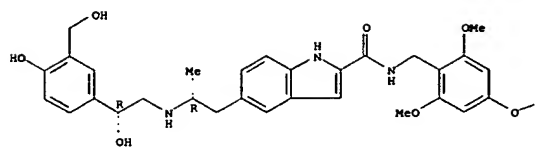
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Title compds. (I: n = 0-4; R<sub>1</sub>, R<sub>2</sub> = H, alkyl; R<sub>3</sub> = H, (un)substituted alkyl; R<sub>4</sub>-R<sub>8</sub> = H, OH, alkyl, alkoxy, hydroxyalkyl, thioalkyl, halo, trifluoromethyl, benzyloxy; their pharmaceutically acceptable salts and/or isomers, tautomers, solvates or isotopic variations), were prepared as  $\beta$ 2 adrenergic receptor agonists. Thus, 5-[(2R)-2-[(2R)-2-[[tert-butyl]dimethylsilyloxy]-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-1H-indole-2-carboxylic acid (preparation given) 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride, hydroxybenzotriazole, and 2-methoxybenzylamine were stirred 18 h in DMF to give the silyl-protected amide derivative. This was stirred with NH<sub>4</sub>F in MeOH/H<sub>2</sub>O to give 5-[(2R)-2-[(2R)-2-[[tert-butyl]dimethylsilyloxy]-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-(2-methoxybenzyl)-1H-indole-2-carboxamide. I showed a  $\beta$ 2 cAMP EC<sub>50</sub> = 0.02-4 nM. I are useful for treating inflammatory, allergic and respiratory diseases.  
IT 679427-60-2P, 5-[(2R)-2-[(2R)-2-Hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-(4-benzyloxy-2,6-dimethoxybenzyl)-1H-indole-2-carboxamide  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
( $\beta$ 2 adrenergic receptor agonist; preparation of indolecarboxamides as  $\beta$ 2 adrenergic receptor agonists)  
RN 679427-60-2 CAPLUS  
CN 1H-Indole-2-carboxamide,  
N-[(2,6-dimethoxy-4-(phenylmethoxy)phenyl)methyl]-  
5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)  
Absolute stereochemistry.

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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IT 677026-80-1P 677026-81-2P 677026-82-3P  
677026-83-4P 677026-84-5P 679427-58-8P.

5-[ (2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(2,4-dichlorobenzyl)-1H-indole-2-carboxamide  
679427-59-99, 5-[ (2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-

hydroxymethylphenyl]yl]amino]propyl]-N-(3-(hydroxy-2,6-dimethoxybenzyl)-1H-indole-2-carboxamide 679427-41-3P, 5-[(2R)-2-[[[2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(4-hydroxy-2,6-dimethoxybenzyl)-1H-indole-2-carboxamide 679427-62-4P, 679427-63-5P, 5-[(2R)-2-[[[2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(2-hydroxy-6-methoxybenzyl)-1H-indole-2-carboxamide 679427-64-6P, 5-[(2R)-2-[[[2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(2-[6-qi]lorobenzyloxy)-1H-indole-2-carboxamide 679427-65-7P,

5-[ (2R)-2-[( (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl)amino]propyl]-N-(2-chlorobenzyl)-1H-indole-2-carboxamide 679427-66-8P,

5-[ (2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl-N-(2-fluorobenzyl)-1H-indole-2-carboxamide 679427-67-99.

5-({(2R)-2-({(2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl}amino)propyl}-N-(4-hydroxybenzyl)-1H-indole-2-carboxamide 679427-68-0P

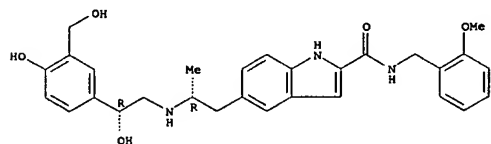
5-[(2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amin  
olopropyl-N-(3-hydroxybenzyl)-1H-indole-2-carboxamide 679427-69-1P

5-((2R)-2-(((2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl)amin

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
( $\beta_2$  adrenergic receptor agonist; prepn. of indolecarboxamides as  
 $\beta_2$  adrenergic receptor agonists)

RN 677026-80-1 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(2-methoxyphenyl)methyl]-  
(9CI) (CA INDEX NAME)

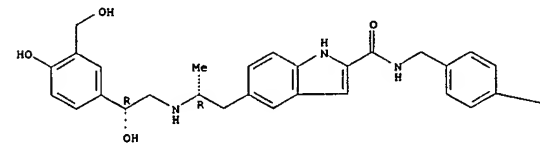
**Absolute stereochemistry.**



RN 677026-81-2 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-[[{2R}-2-[[{2R}-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

**Absolute stereochemistry.**

PAGE 1-A



PAGE 1-B



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RN      677026-82-3  CAPLUS
CN      1H-Indole-2-carboxamide,
N-[(2,6-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-
      2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI)
      (CA INDEX NAME)

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L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 olpropyl]-N-(2-methylsulfonylbenzyl)-1H-indole-2-carboxamide  
 679427-70-4P, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-  
 hydroxymethylphenyl)ethyl]amino]propyl]-N-(4-methylsulfonylbenzyl)-  
 indole-2-carboxamide 679427-71-5P, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-  
 hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(2,3-  
 dimethoxybenzyl)-1H-indole-2-carboxamide 679427-72-6P,

5-[(2R)-2-{[(2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino}propyl]-N-(2,4-dimethoxybenzyl)-1H-indole-2-carboxamide  
679427-73-7F, 5-[(2R)-2-{[(2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino}propyl]-N-(2-ethoxybenzyl)-1H-indole-2-carboxamide 679427-74-8F, 5-[(2R)-2-{[(2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino}propyl]-N-benzyl-N-methyl-1H-indole-2-carboxamide 679427-75-8F, 5-[(2R)-2-{[(2R)-2-Hydroxy-2-

4-(4-hydroxy-3-hydroxymethylphenyl)ethylaminopropyl-N-benzyl-1H-indole-2-carboxamide 67942-76-05, 5-[(2R)-2-[(1R)-2-hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethylamino]propyl]-N-(4-fluorobenzyl)-1H-indole-2-carboxamide 67942-77-1P, 5-[(2R)-2-[(1R)-2-hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethylamino]propyl]-N-(2-methoxy-3-methylbenzyl)-1H-indole-2-carboxamide 67942-78-2P,

5-[(2R)-2-[(2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(3-methoxy-2-methylbenzyl)-1H-indole-2-carboxamide  
679427-79-3P, 1-Ethyl-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-

hydroxymethylphenyl)ethyl]amino]propyl)-N-(2-[6-dimethoxybenzyl]-1H-indole-2-carboxamide **679427-80-6P**, 1-Ethyl-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl)-N-(2-methoxybenzyl)-1H-indole-2-carboxamide **679427-81-7P**, 1-Ethyl-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl)-N-(4-chlorobenzyl)-1H-indole-2-carboxamide **679427-82-6P**, 1-Methyl-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-

hydroxymethylphenyl)ethyl]amino]propyl]-N-(2,6-dimethoxybenzyl)-1H-indole-2-carboxamide 679427-83-9P, 1-Methyl-5-[(2R)-2-[(2R)-2-hydroxy-

2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(2-methoxybenzyl)-1H-indole-2-carboxamide 679427-84-0P, 1-Methyl-5-[[2(R)-2-[[2(R)-2-hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]propyl]-N-(4-chlorobenzyl)-1H-indole-2-carboxamide 679427-85-1P.

5-[(2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]butyl]-N-(2-methoxybenzyl)-1H-indole-2-carboxamide 679427-86-2P.

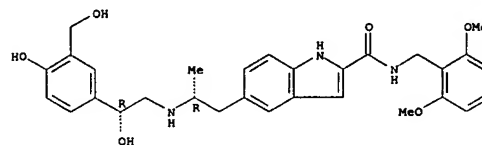
5-[(2R)-2-[[[(2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]butyl]-N-(2,6-dimethoxybenzyl)-1H-indole-2-carboxamide

679427-87-3P, 5-[ (2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]butyl]-N-(2-ethoxybenzyl)-1H-indole-2-carboxamide 679427-88-4P, 5-[ (2R)-2-[[ (2R)-2-Hydroxy-2-(4-hydroxy-3-hydroxymethylphenyl)ethyl]amino]butyl]-N-benzyl-1H-indole-2-carboxamide

carboxamide  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

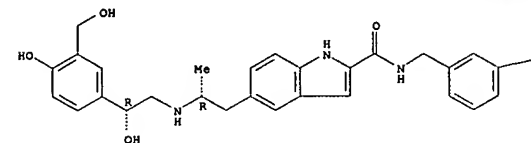
**Absolute stereochemistry.**



RN 677026-83-4 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(3-methoxyphenyl)methyl]-  
(9CI) (CA INDEX NAME)

**Absolute stereochemistry.**

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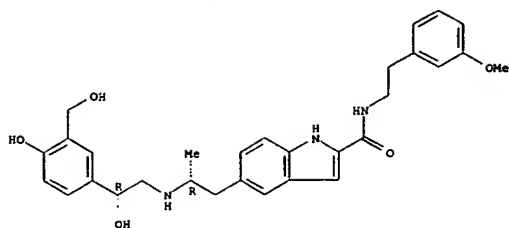
PAGE 1-B



RN 677026-84-5 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[[2R)-2-[[[2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[2-(3-methoxyphenyl)ethyl]-  
(9CI) [CA INDEX NAME]

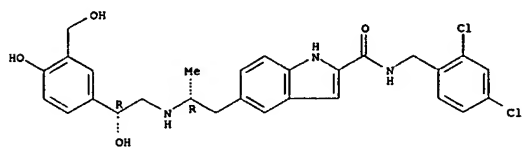
**Absolute stereochemistry.**

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 679427-58-8 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2,4-dichlorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

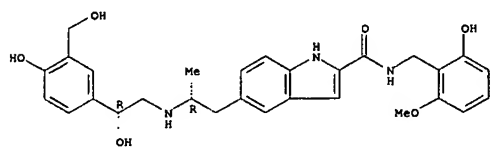


RN 679427-59-9 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(3-hydroxy-2,6-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

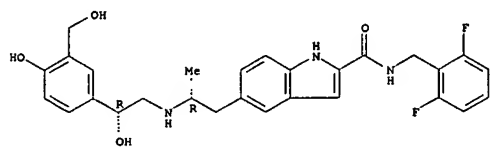
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



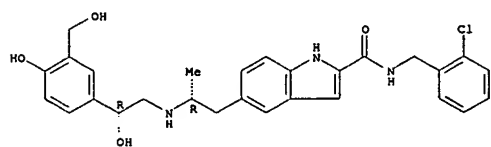
RN 679427-64-6 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2,6-difluorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



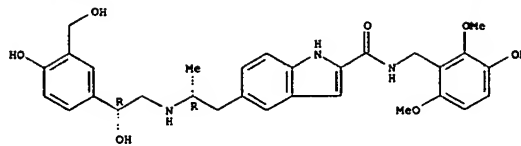
RN 679427-65-7 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2-chlorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



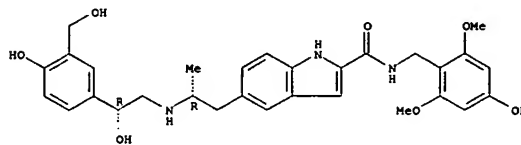
RN 679427-66-8 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2-fluorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



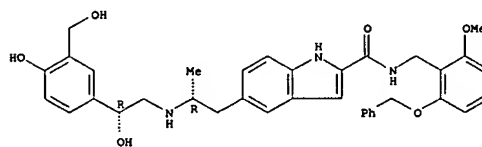
RN 679427-61-3 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(4-hydroxy-2,6-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 679427-62-4 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2-methoxy-6-phenylmethoxy)phenyl]methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

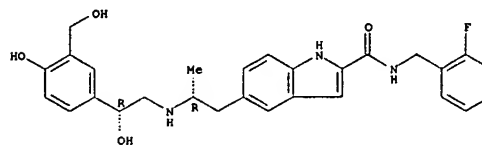


RN 679427-63-5 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2-methoxy-6-phenylmethoxy)phenyl]methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

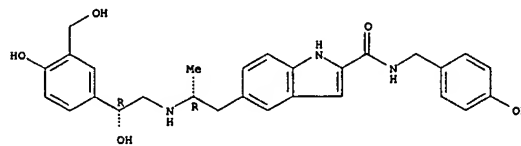
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



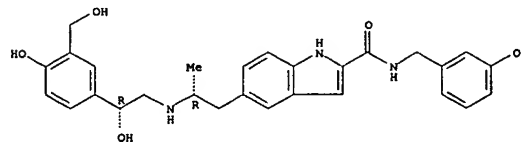
RN 679427-67-9 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2,6-difluorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 679427-68-0 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2,6-difluorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

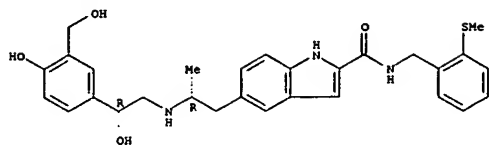


RN 679427-69-1 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[(2-methylthio)phenyl]methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.

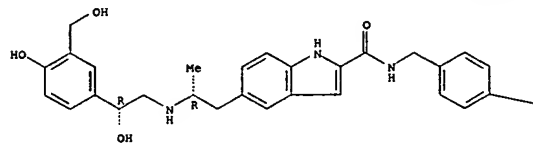


RN 679427-70-4 CAPLUS

CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-[(4-(methylthio)phenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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PAGE 1-B

SMe

RN 679427-71-5 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(2,3-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

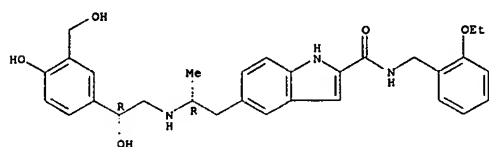
Absolute stereochemistry.

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 679427-73-7 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(2-ethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

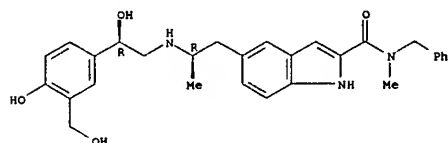
Absolute stereochemistry.



RN 679427-74-8 CAPLUS

CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

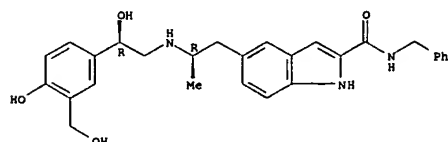
Absolute stereochemistry.



RN 679427-75-9 CAPLUS

CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

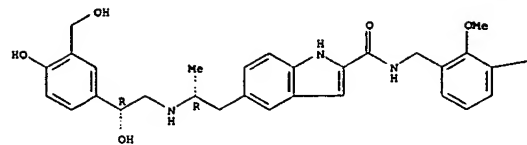
Absolute stereochemistry.



RN 679427-76-0 CAPLUS

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

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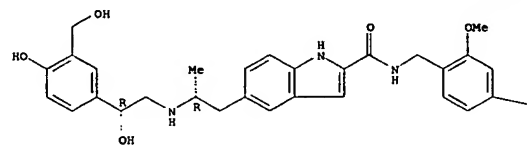
OMe

RN 679427-72-6 CAPLUS

CN 1H-Indole-2-carboxamide, N-[(2,4-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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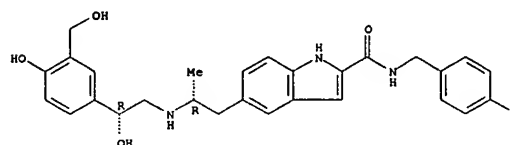
PAGE 1-B

OMe

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CN 1H-Indole-2-carboxamide, N-[(4-fluorophenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]- (9CI) (CA INDEX NAME)

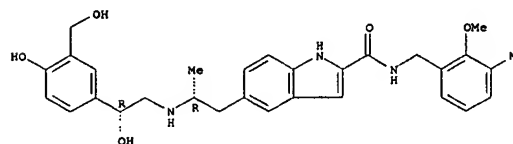
Absolute stereochemistry.



RN 679427-77-1 CAPLUS

CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-[(2-methoxy-3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

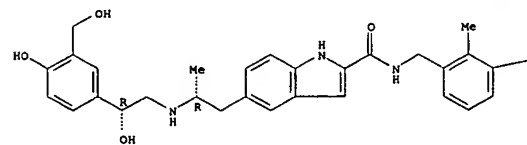


RN 679427-78-2 CAPLUS

CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-(4-hydroxy-3-(hydroxymethyl)phenyl)ethyl]amino]propyl]-N-[(3-methoxy-2-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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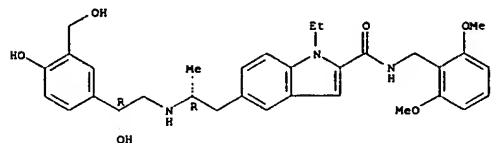
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
PAGE 1-B

—OMe

RN 679427-79-3 CAPLUS  
CN 1H-Indole-2-carboxamide,  
N-[(2,6-dimethoxyphenyl)methyl]-1-ethyl-5-[(2R)-2-

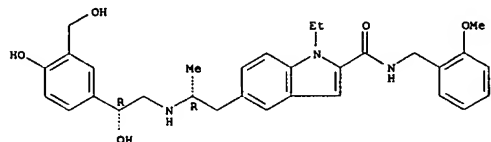
[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-1-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 679427-80-6 CAPLUS  
CN 1H-Indole-2-carboxamide,  
1-ethyl-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(2-methoxyphenyl)methyl]-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

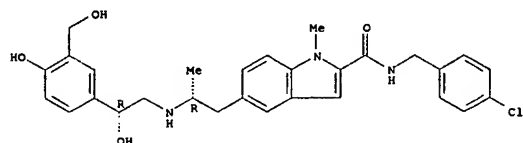


RN 679427-81-7 CAPLUS  
CN 1H-Indole-2-carboxamide, N-[(4-chlorophenyl)methyl]-1-ethyl-5-[(2R)-2-  
[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-  
(9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

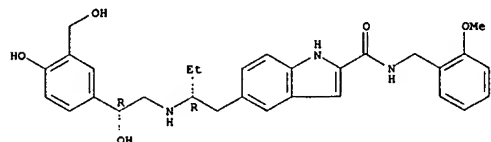
hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-1-methyl-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



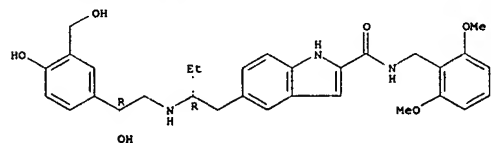
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CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]butyl]-N-[(2-methoxyphenyl)methyl]-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



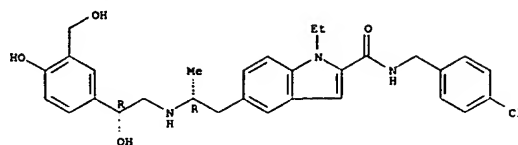
RN 679427-86-2 CAPLUS  
CN 1H-Indole-2-carboxamide,  
N-[(2,6-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]butyl]-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



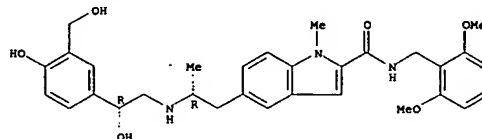
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CN 1H-Indole-2-carboxamide, N-[(2-ethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
Absolute stereochemistry.



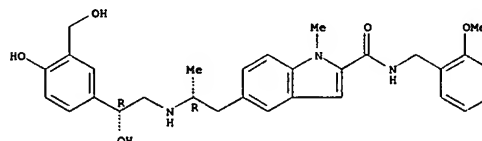
RN 679427-82-8 CAPLUS  
CN 1H-Indole-2-carboxamide,  
N-[(2,6-dimethoxyphenyl)methyl]-5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-1-  
methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 679427-83-9 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl]-N-[(2-methoxyphenyl)methyl]-1-  
methyl- (9CI) (CA INDEX NAME)

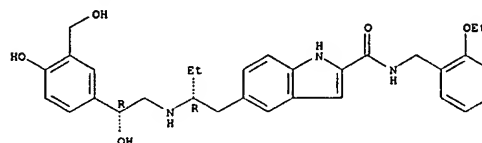
Absolute stereochemistry.



RN 679427-84-0 CAPLUS  
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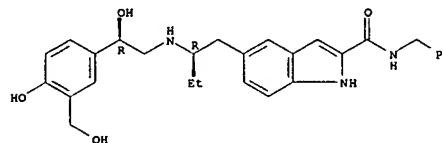
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]butyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



RN 679427-88-4 CAPLUS  
CN 1H-Indole-2-carboxamide, 5-[(2R)-2-[(2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]butyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

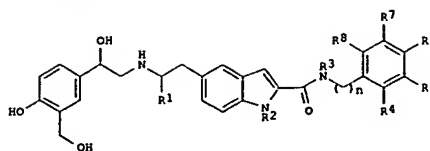
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:305136 CAPLUS  
 DOCUMENT NUMBER: 140:303532  
 TITLE: Preparation of indolecarboxamides as  $\beta 2$  adrenergic receptor agonists  
 INVENTOR(S): Brown, Alan; Bryans, Justin; Bunnage, Mark Edward; Glossop, Paul Alan; Lane, Charlotte; Mantell, Simon  
 PATENT ASSIGNEE(S): Pfizer Limited, UK  
 SOURCE: Eur. Pat. Appl., 32 pp.  
 CODEN: EPKXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

*Inventors*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1407769	A1	20040414	EP 2002-292513	20021011
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CA 2499314	AA	20040422	CA 2003-2499314	20031006
WO 2004032921	A1	20040422	WO 2003-1B4441	20031006
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, BF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1356034	A1	20050727	EP 2003-751095	20031006
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BR 2003015234	A	20050823	BR 2003-15234	20031006
US 2004116503	A1	20040617	US 2003-684233	20031009
US 6844362	B2	20050118		
US 2005085226	A1	20050421	US 2004-959934	20041005
NO 2005001406	A	20050422	NO 2005-1406	20050317
PRIORITY APPLN. INFO.			EP 2002-292513	A 20021011
			US 2003-438639P	P 20030108
			EP 2003-290069	A 20030110
			WO 2003-1B4441	W 20031006
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OTHER SOURCE(S): MARPAT 140:303532  
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L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

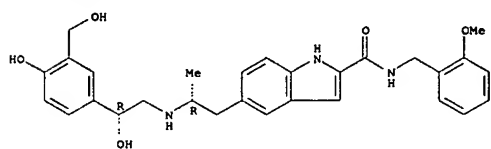


AB Title compds. (I; n = 0-4; R1, R2 = H, alkyl; R3 = H, alkyl, hydroxyalkyl; R4-R8 = H, OH, alkyl, alkoxy, hydroxyalkyl, thioalkyl, halo, trihalomethyl), were prepared Thus, 5-((2R)-2-((2R)-2-[[tert-butyl(dimethylsilyl)oxy]-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)-1H-indole-2-carboxylic acid (preparation given) 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride, hydroxybenzotriazole, and 2-methoxybenzylamine were stirred 18 h in DMF to give the silyl-protected amide derivative This was stirred with NH4F in MeOH/H2O to give 5-((2R)-2-((2R)-2-[[tert-butyl(dimethylsilyl)oxy]-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)-N-(2-methoxybenzyl)-1H-indole-2-carboxamide. I showed a  $\beta 2$  cAMP EC50 = 0.02-0.9 nM. The indole derivs. according to the present invention are useful in numerous diseases, disorders and conditions, in particular inflammatory, allergic and respiratory diseases, disorders and conditions.

IT 677026-80-1P 677026-81-2P 677026-82-3P  
 677026-83-4P 677026-84-5P  
 RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (claimed compound; preparation of indolecarboxamides as  $\beta 2$  adrenergic receptor agonists)  
 RN 677026-80-1 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-((2R)-2-((2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)-N-((2-methoxyphenyl)methyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

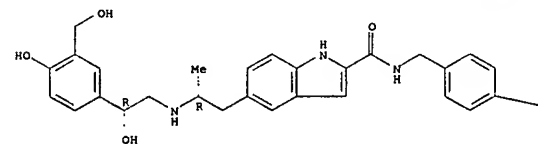
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 677026-81-2 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-((2R)-2-((2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)-N-((4-(trifluoromethyl)phenyl)methyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



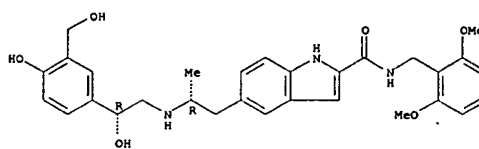
PAGE 1-B

CF3

RN 677026-82-3 CAPLUS  
 CN 1H-Indole-2-carboxamide, N-[[2,6-dimethoxyphenyl)methyl]-5-((2R)-2-((2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

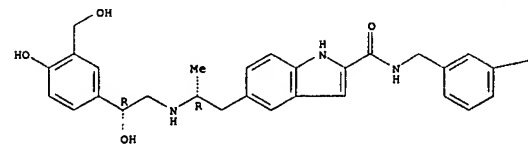
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 677026-83-4 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-((2R)-2-((2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)-N-((3-methoxyphenyl)methyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



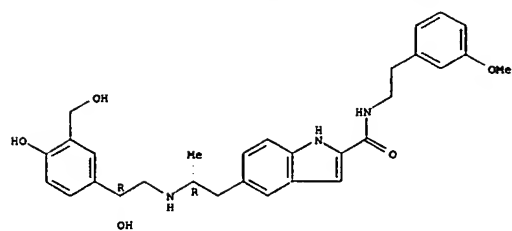
PAGE 1-B

OMe

RN 677026-84-5 CAPLUS  
 CN 1H-Indole-2-carboxamide, 5-((2R)-2-((2R)-2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]propyl)-N-2-((3-methoxyphenyl)ethyl)- (9CI) (CA INDEX NAME)

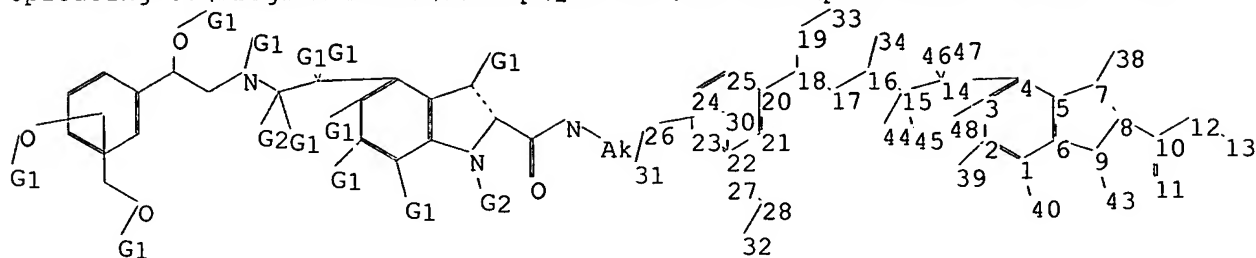
Absolute stereochemistry.

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

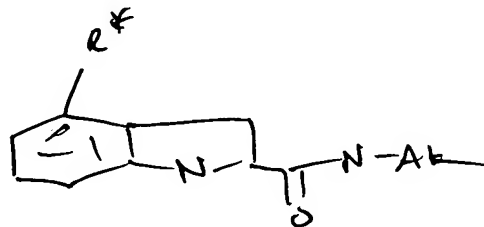


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Uploading C:\Program Files\Stnexp\Queries\10813426\positional isomer 1.str



positional isomer



chain nodes :

10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 38 39 40 43  
44 45 46 47 48

ring nodes :

1 2 3 4 5 6 7 8 9 20 21 22 23 24 25

chain bonds :

1-40 2-39 3-48 4-14 7-38 8-10 9-43 10-11 10-12 12-13 14-15 14-47 14-46  
15-16 15-44 15-45 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24  
24-25

exact/norm bonds :

1-40 2-39 3-48 5-7 6-9 7-8 7-38 8-9 9-43 10-11 10-12 12-13 14-47 14-46  
15-16 15-44 15-45 16-17 16-34 18-19 19-33 26-31 27-28 28-32

exact bonds :

4-14 8-10 14-15 17-18 18-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 20 :

G1:H,CH3

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS  
 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 38:CLASS  
 39:CLASS 40:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS

L4        STRUCTURE UPLOADED

=> s l4

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:01:19 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -        195 TO ITERATE

100.0% PROCESSED        195 ITERATIONS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                              BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:        3063 TO        4737  
PROJECTED ANSWERS:            0 TO        0

0 ANSWERS

L5            0 SEA SSS SAM L4

L6            0 L5

=> s l4 full

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 09:01:24 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED -        3846 TO ITERATE

100.0% PROCESSED        3846 ITERATIONS  
SEARCH TIME: 00.00.01

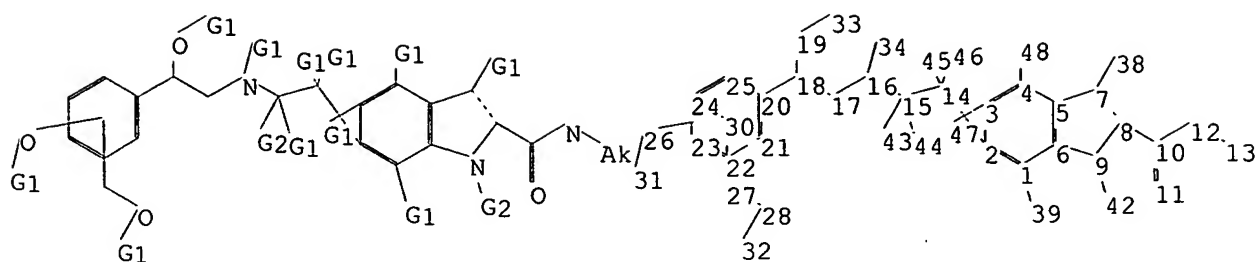
L7            0 SEA SSS FUL L4

L8            0 L7

=>

Uploading C:\Program Files\Stnexp\Queries\10813426\positional isomer 2.str

0 ANSWERS



positional isomer.



chain nodes :

10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 38 39 42 43  
44 45 46 47 48

ring nodes :

1 2 3 4 5 6 7 8 9 20 21 22 23 24 25

chain bonds :

1-39 2-14 3-47 4-48 7-38 8-10 9-42 10-11 10-12 12-13 14-15 14-46 14-45  
15-16 15-43 15-44 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24  
24-25

exact/norm bonds :

1-39 3-47 4-48 5-7 6-9 7-8 7-38 8-9 9-42 10-11 10-12 12-13 14-46 14-45  
15-16 15-43 15-44 16-17 16-34 18-19 19-33 26-31 27-28 28-32

exact bonds :

2-14 8-10 14-15 17-18 18-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 20 :

G1:H,CH3

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS  
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 38:CLASS  
39:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS

L9 STRUCTURE UPLOADED

=&gt; s 19 full

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 09:02:22 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 81734 TO ITERATE

100.0% PROCESSED 81734 ITERATIONS  
 SEARCH TIME: 00.00.11

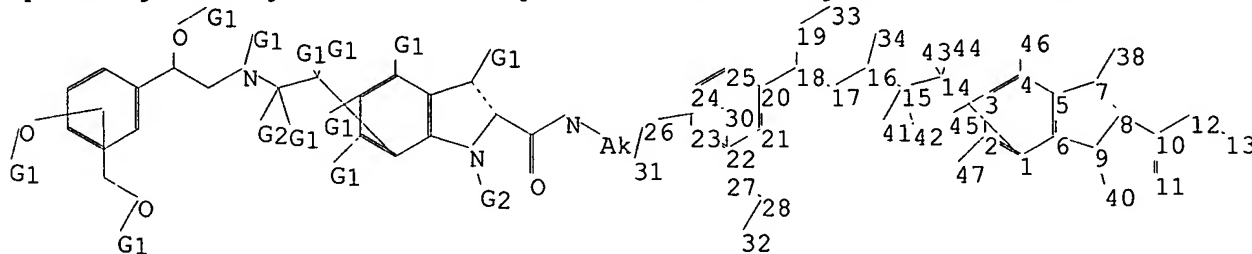
0 ANSWERS

L10 0 SEA SSS FUL L9

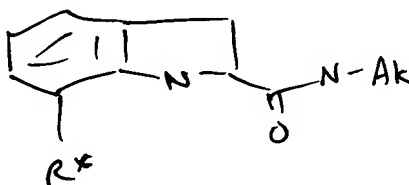
L11 0 L10

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Uploading C:\Program Files\Stnexp\Queries\10813426\positional isomer 3.str



positional isomer



chain nodes :

10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 38 40 41 42  
 43 44 45 46 47

ring nodes :

1 2 3 4 5 6 7 8 9 20 21 22 23 24 25

chain bonds :

1-14 2-47 3-45 4-46 7-38 8-10 9-40 10-11 10-12 12-13 14-15 14-44 14-43  
 15-16 15-41 15-42 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24  
 24-25

exact/norm bonds :



2-47 3-45 4-46 5-7 6-9 7-8 7-38 8-9 9-40 10-11 10-12 12-13 14-44 14-43  
15-16 15-41 15-42 16-17 16-34 18-19 19-33 26-31 27-28 28-32

exact bonds :

1-14 8-10 14-15 17-18 18-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 20 :

G1:H,CH3

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS

28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 38:CLASS

40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS

L12 STRUCTURE UPLOADED

=> s l12 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 09:03:26 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 144106 TO ITERATE

100.0% PROCESSED 144106 ITERATIONS  
SEARCH TIME: 00.00.13

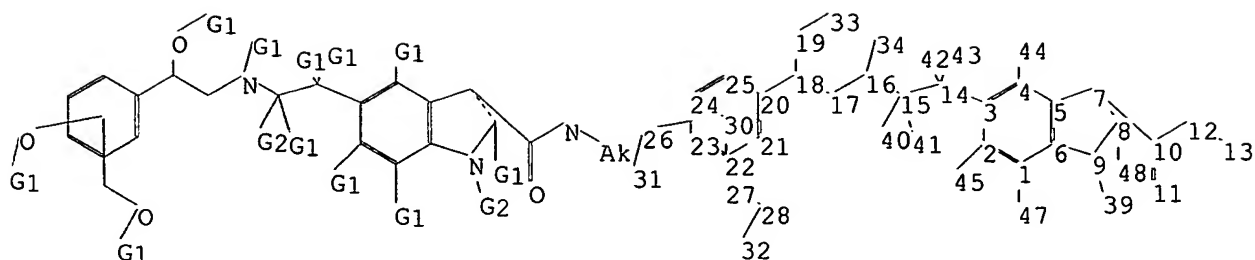
0 ANSWERS

L13 0 SEA SSS FUL L12

L14 0 L13

=>

Uploading C:\Program Files\Stnexp\Queries\10813426\positional isomer 4.str



positional isomer



chain nodes :

10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 39 40 41 42  
43 44 45 47 48

ring nodes :

1 2 3 4 5 6 7 8 9 20 21 22 23 24 25

chain bonds :

1-47 2-45 3-14 4-44 7-10 8-48 9-39 10-12 10-11 12-13 14-15 14-43 14-42  
15-16 15-40 15-41 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24  
24-25

exact/norm bonds :

1-47 2-45 4-44 5-7 6-9 7-8 8-9 8-48 9-39 10-12 10-11 12-13 14-43 14-42  
15-16 15-40 15-41 16-17 16-34 18-19 19-33 26-31 27-28 28-32

exact bonds :

3-14 7-10 14-15 17-18 18-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 20 :

G1:H,CH3

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS  
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 39:CLASS  
40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 47:CLASS 48:CLASS

L15      STRUCTURE UPLOADED

=> s l15 full

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 09:04:47 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED -      483 TO ITERATE

100.0% PROCESSED      483 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L16      0 SEA SSS FUL L15

L17      0 L16

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	855.70
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

STN INTERNATIONAL LOGOFF AT 09:05:05 ON 25 JAN 2006

0.21

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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STRUCTURE FILE UPDATES:    24 JAN 2006  HIGHEST RN 872575-89-8
DICTIONARY FILE UPDATES:  24 JAN 2006  HIGHEST RN 872575-89-8
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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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*
* The CA roles and document type information have been removed from
* the IDE default display format and the ED field has been added,
* effective March 20, 2005.  A new display format, IDERL, is now
* available and contains the CA role and document type information.
*
*****
```

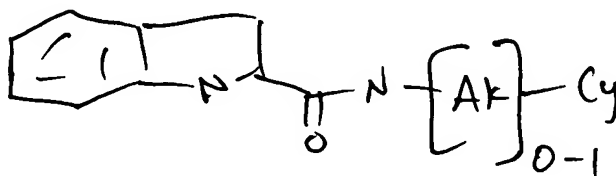
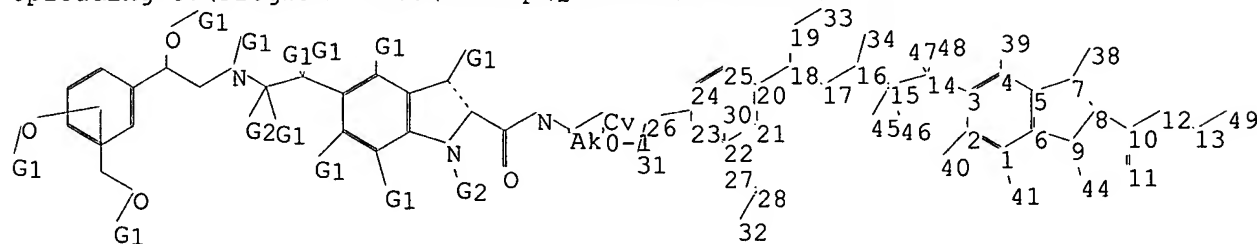
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

 $\Rightarrow$ 

Uploading C:\Program Files\Stnexp\Queries\10813426\4.str



↙ Q can be a single bond

```

chain nodes :
10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 38 39 40 41
44 45 46 47 48 49
ring nodes :
1 2 3 4 5 6 7 8 9 20 21 22 23 24 25
chain bonds :
1-41 2-40 3-14 4-39 7-38 8-10 9-44 10-11 10-12 12-13 13-49 14-15 14-47
14-48 15-16 15-45 15-46 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28
28-32
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24
24-25
exact/norm bonds :
1-41 2-40 4-39 5-7 6-9 7-8 7-38 8-9 9-44 10-11 10-12 12-13 13-49 14-47
14-48 15-16 15-45 15-46 16-17 16-34 18-19 19-33 26-31 27-28 28-32
exact bonds :
3-14 8-10 14-15 17-18 18-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25
isolated ring systems :
containing 20 :

```

G1:H,CH3

G2:H,Ak

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 38:CLASS
39:CLASS 40:CLASS 41:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS
49:Atom

```

L1 STRUCTURE UPLOADED

```

=> s l1 full
FULL SEARCH INITIATED 09:20:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 80161 TO ITERATE

```

```

100.0% PROCESSED 80161 ITERATIONS
SEARCH TIME: 00.00.11

```

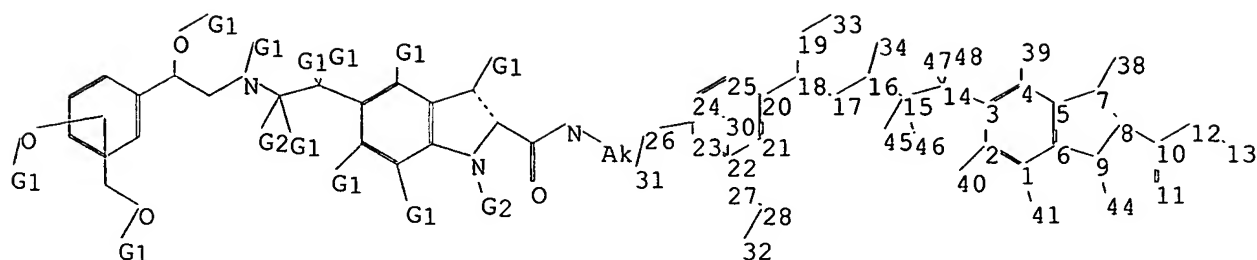
54 ANSWERS

L2 54 SEA SSS FUL L1

```

=>
Uploading C:\Program Files\Stnexp\Queries\10813426\3.str

```



chain nodes :

10 11 12 13 14 15 16 17 18 19 26 27 28 31 32 33 34 38 39 40 41  
44 45 46 47 48

ring nodes :

1 2 3 4 5 6 7 8 9 20 21 22 23 24 25

chain bonds :

1-41 2-40 3-14 4-39 7-38 8-10 9-44 10-11 10-12 12-13 14-15 14-47 14-48  
15-16 15-45 15-46 16-17 16-34 17-18 18-19 18-20 19-33 26-31 27-28 28-32

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 20-21 20-25 21-22 22-23 23-24  
24-25

exact/norm bonds :

1-41 2-40 4-39 5-7 6-9 7-8 7-38 8-9 9-44 10-11 10-12 12-13 14-47 14-48  
15-16 15-45 15-46 16-17 16-34 18-19 19-33 26-31 27-28 28-32

exact bonds :

3-14 8-10 14-15 17-18 18-20

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 20-21 20-25 21-22 22-23 23-24 24-25

isolated ring systems :

containing 20 :

G1:H,CH3

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS  
28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 38:CLASS  
39:CLASS 40:CLASS 41:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS

L3 STRUCTURE UPLOADED

=> s 13 full

FULL SEARCH INITIATED 09:21:32 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 80161 TO ITERATE

100.0% PROCESSED 80161 ITERATIONS  
SEARCH TIME: 00.00.10

54 ANSWERS

L4 54 SEA SSS FUL L3

=&gt; s l2 or l4

L5 54 L2 OR L4

=&gt; fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

336.08

336.29

FILE 'CAPLUS' ENTERED AT 09:24:00 ON 25 JAN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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<http://www.cas.org/infopolicy.html>

=&gt; s l2 or l4

3 L2

3 L4

L6

3 L2 OR L4

=&gt;

---Logging off of STN---

=&gt;

Executing the logoff script...

=&gt; LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.46

336.75

← crossed w/ original str.

} same hits - nothing new  
when Q=0